

## On the Constancy of Self-Diffusion Coefficient at the Solid-Liquid Phase Transition

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An analytical method for calculation of the vacancy and diffusional parameters in the isotropic lattice model, in which part of the cells are vacated and others are occupied with spherical atoms is proposed. The atoms in the system can be either in localization state or in delocalization. This model may be used for the description of both solid and liquid and gas phases. By means of this method we studied the solid-liquid phase transition into FCC and BCC metals.

The relationship is obtained between delocalization energy ( $E_d$ ) and vacancy formation's energy ( $E_v$ ) into the virtual lattice, where part of atoms are delocalized

$$E_v / k_b T = (2 \pi^2 k_y^{2/3} E_d / k_b T) / 3k_{no} \{1 + x[(8 \pi^2 E_d / 9k_b T) \bar{n} - 1]\},$$

where  $k_b$  is the Boltzmann's constant,  $T$  is the temperature,  $x$  is the fraction of delocalized atoms (it is defined by value  $E_d / k_b T$  only),  $k_y$  is the packing fraction coefficient for virtual lattice of  $N+N_v$  spherical cell,  $k_{no}$  is the number of nearest-neighbour (both occupied and vacated) cell (i.e. it is the first coordinational number into virtual lattice model, where  $N$  cell are occupied by atoms, and  $N_v$  cell are vacated).

Thus, both diffusional parameters and vacancy parameters are defined by one the same argument:  $E_d / k_b T$ . Therefore the delocalization of atoms in a crystal is connected with the vacancy formation's process in it. Evaluations are shown that for solid phase along the melting curve the fraction of vacant cell ( $\phi_s$ ), the fraction of delocalized atoms ( $x_s$ ) and the diffusion coefficient are approximately constants for simple monatomic matters with the same crystal structure. For the metals with FCC (first line) and BCC (second line) structures are obtained:

$$\begin{array}{lll} \phi_s = 3.7 * 10^{-3} ; & x_s = 2.87 * 10^{-4} ; & D_s / [ \text{cm}^2 / \text{c} ] = 2.86 * 10^{-7} ; \\ \phi_s = 3.7 * 10^{-3} ; & x_s = 3.84 * 10^{-4} ; & D_s / [ \text{cm}^2 / \text{c} ] = 3.84 * 10^{-6} . \end{array}$$

For the liquid phase along the melting curve the constancy of above-mentioned parameters also is observed (although it is more approximate than for the solid phase). At the crystallization of liquid phase of simple materials with FCC (first line) and BCC (second line) virtual structures the above-mentioned values are equal:

$$\begin{array}{lll} \phi_l = 0.1 \div 0.2 ; & x_l = (2.4 \div 4.8) * 10^{-2} ; & D_l / [ \text{cm}^2 / \text{c} ] = (2 \div 4) * 10^{-5} ; \\ \phi_l = 0.1 \div 0.2 ; & x_l = (3.7 \div 7.2) * 10^{-2} ; & D_l / [ \text{cm}^2 / \text{c} ] = (3 \div 7) * 10^{-5} . \end{array}$$

It should be noted that melting of crystal is due to delocalization of atoms, but it is not by activation of various structure defects. The origin of S-loop at the isotherm of state equation  $P(V)$  into the melting region is due to the sharp growth of function  $x(V)$ , i.e. it is due to the sharp delocalization of atoms if the volume of the system is larger than some value. The formation of structure vacancies into the lattice is a consequence of the delocalization of atoms, when their kinetic energy reaches some critical value. Therefore the constancy of value  $x_s$  (or  $x_l$ ) involves the constancy of value  $\phi_s$  (or  $\phi_l$ ) for a given crystal structure. Instability of a given crystal lattice is observed at the critical values  $x_s$  and  $\phi_s$  and agrees with the results of "percolation theory".